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# MOLECULAR DYNAMICS SIMULATIONS OF THE BACKSCATTERING OF $He^{++}$ IONS FROM A RANDOM ASSEMBLY OF GOLD ATOMS

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The backscattering of 8 - 50 keV $He^{++}$ from uniformly distributed Au atoms is investigated with a computer code based on the Molecular Dynamics method. A screened Coulomb type potential is used to describe the interactions between particles. The angular distribution, the energy - loss and energy distributions of backscattered particles are calculated using two different energy - loss models: the Lindhard - Scharff nonlocal energy loss and the Firsov model. The energy - loss distribution presents a peak for 30 keV incident energy for both models, whereas other incident energies show a cvasi - continuous spectrum. The energy distribution indicates Binary Collision Approximation (BCA) is approximately verified for 8 and 20 keV for the Lindhard - Scharff model and for 8, 20, and 30 keV for the Firsov model.

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## 1. Introduction

For energies below 50 keV the scattering of ions in solids is governed by multiple collisions [1]. Due to the complexity of the backscattering process in this energy range, various approaches were developed. It is well known that Molecular Dynamics (MD) simulations, based on numerical integration of the equations of motion, provide more realistic descriptions of collision processes, but at the expense of a greater computational time [2]. The first aim of this paper is to estimate the angular distribution, the energy - loss and energy distributions of 8 - 50 keV $He^{++}$ ions backscattered from a Au target consisting in a random assembly of 5900 atoms, at normal incidence. The second aim is to compare the influence of two inelastic energy loss models: the Lindhard – Scharff (LS) nonlocal energy loss model and the Firsov model.

## 2. Model

The MD model is based on a screened - Coulomb type potential of the form [3]:

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \Phi\left(\frac{r}{a}\right) \tag{1}$$

with $\Phi(r/a)$ approximated by:

$$\Phi\left(\frac{r}{a}\right) = \sum_{i=1}^{n} c_i \exp(-d_i \frac{r}{a}), \qquad \sum_{i=1}^{n} c_i = \Phi(0) = 1 \tag{2}$$

the screening length $a$ depending on $Z_1$ and $Z_2$ . The usual ansatz $Z_{12} = (Z_1^x + Z_2^x)^y$ transforms the screening length in:

$$a = \left(\frac{9\pi^2}{128}\right)^{1/3} a_B Z_{12}^{-1/3} \tag{3}$$

with $a_B$ the Bohr radius. Following Firsov [4], we use x = 1/2 and y = 2.

The constants $c_i$ and $d_i$ are listed in the table below (Table 1) and yield the ZBL (Ziegler-Biersack-Littmark) potential [4].

Table 1. The constants of the screened – Coulomb potential.

| | | | | |
|---|---|---|---|---|
| $c_i$, i = 1,4 | 0.028171 | 0.28022 | 0.50986 | 0.18175 |
| $d_i$, i = 1,4 | 0.20162 | 0.40290 | 0.94229 | 3.1998 |

The incident beam is formed by $4 \times 10^3$ $He^{++}$ ions, normally incident on a 10 × 100 × 100 Angstroms Au target, containing 5900 randomly distributed atoms with the density 0.59 atoms/$A^3$. The positions of the Au atoms were computed via a simple random numbers generator. Fig. 1 displays the pair distribution function, which approaches a Gaussian, as expected due to the uniform distribution of the atom positions.

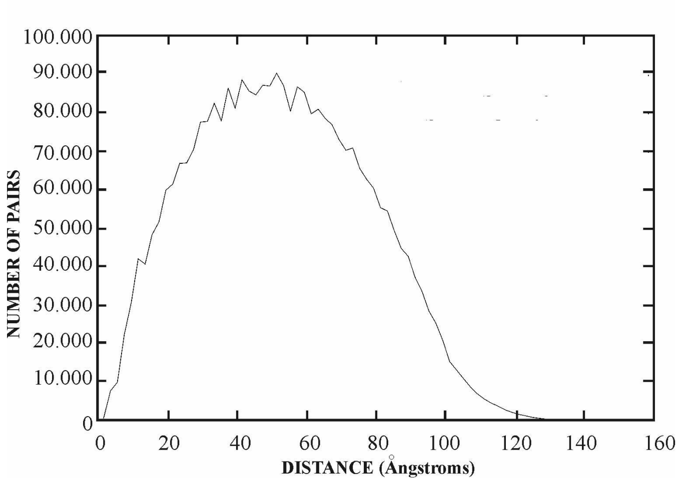


Fig. 1. Atom - atom pair distribution function.

Only the interactions between He ions and Au atoms in a sphere of 4 A radius were considered, at each time step, following the ion trajectory. The time step was chosen in the interval $10^{-16}$ - $10^{-17}$ s, corresponding to incident energies between 8 and 50 keV. The calculations needed approximately 18 hours on a simple Pentium computer.

Two different energy - loss parameterizations were used: the Lindhard - Scharff nonlocal energy loss [5] which is independent of the impact parameter, and the Firsov [6] parameterization (hereafter denoted by F) for the inelastic energy loss as a function of the impact parameter, p, and kinetic energy, E.

In their reference article, Lindhard and Scharff included the loss of energy by considering it to be proportional to the velocity of an ion moving through an electron gas of constant density. Using a Thomas - Fermi [7] treatment for the variation of the stopping cross section per atom with $Z_1$ and $Z_2$, the expression for the energy loss becomes:

$$\Delta E_{LS} = L_m N S_L(E), \qquad S_L = k_L E^{1/2} \tag{4}$$

with:

$$k_L = \frac{1.21 Z_1^{7/6} Z_2}{(Z_1^{2/3} + Z_2^{2/3})^{3/2} M_1^{1/2}} \tag{5}$$

where $L_m$ is the distance between collisions and N = $5.90 \times 10^{22}$ atoms/$cm^3$ for Au.

The basic idea for the derivation of the Firsov's formula is that the energy loss depends on the screening length as:

$$Q \sim \int \Phi^2 dx \tag{6}$$

where Φ is defined by (2). The use of an asymptotic Thomas – Fermi approximation [6] where $\Phi \sim x^{-3}$ gives then $Q \sim x^{-5}$. The final form, by dropping the singularity at x = 0, is:

$$Q(p,E) = \frac{\alpha_{12} E^{1/2}}{(1+\beta_{12} p)^5} \tag{7}$$

with:

$$\alpha_{12} = 0.06685 \frac{(Z_1 + Z_2)^{1/3}}{M_1^{1/2}} and \beta_{12} = 0.3043(Z_1 + Z_2)^{1/3} \tag{8}$$

## 3. Results and discussion

Figs. 2a and 2b show the angular distribution of backscattered particles for Lindhard – Scharff and Firsov energy - loss models, using incident beams of 8, 20, and 30 keV respectively. The straight lines give a cosine distribution. The channel width is Δcosβ = 0.05. The distributions exhibit a similar behavior in deviation from the cosine distribution. More particles are backscattered at large exit angles β(β is the angle between the outgoing particle and the horizontal surface), and fewer particles at small exit angles than for a cosine distribution. Larger departures were observed in both cases for 40 and 50 keV (not shown). Both figures indicate 'preferred' scattering angles between $60^0$ and $70^0$.

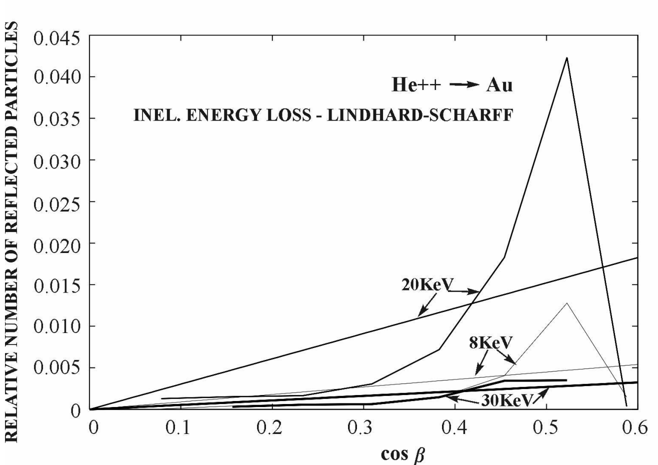


Fig. 2a. Angular distribution of backscattered the $He^{2+}$ particles for incident energies of 8, 20 and 30 keV for Lindhard-Scarff inelastic energy loss. Straight lines represent cosine distributions

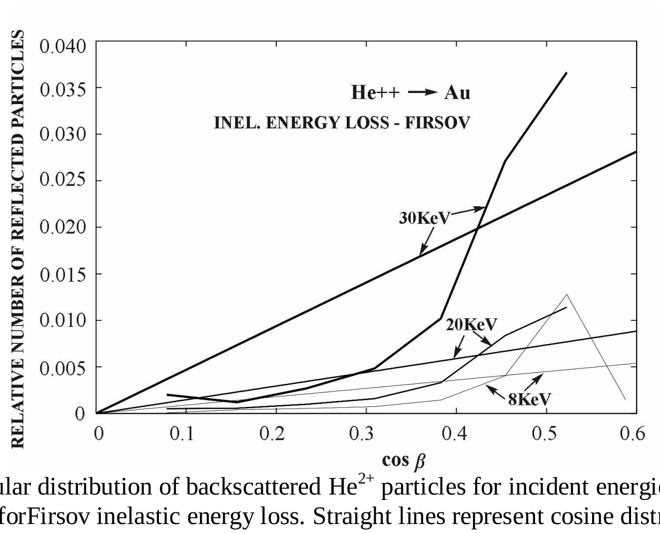


Fig. 2b. Angular distribution of backscattered $He^{2+}$ particles for incident energies of 8, 20 and 30 keV forFirsov inelastic energy loss. Straight lines represent cosine distributions.

In Figs. 3a and 3b it is presented the energy - loss distribution for 8 - 50 keV incident beams for the LS and F models. Both models present a 'peak' corresponding to an incident energy of 30 keV, the other incident values showing a cvasi-continuous spectrum.

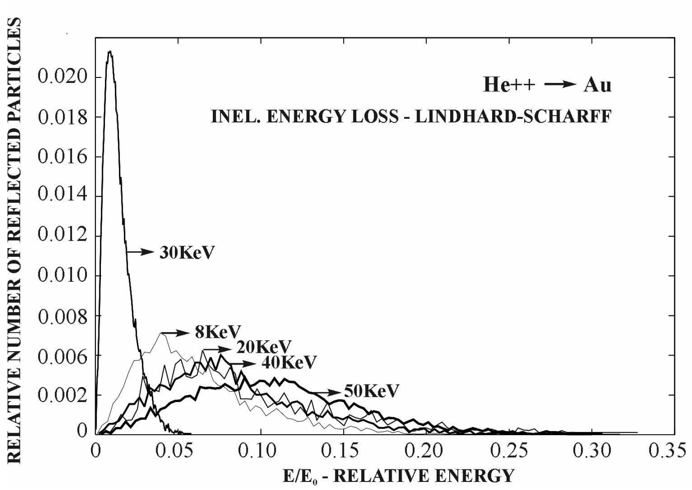


Fig. 3a. Energy distribution of backscattered $He^{2+}$ particles for Lindhard-Scharff.

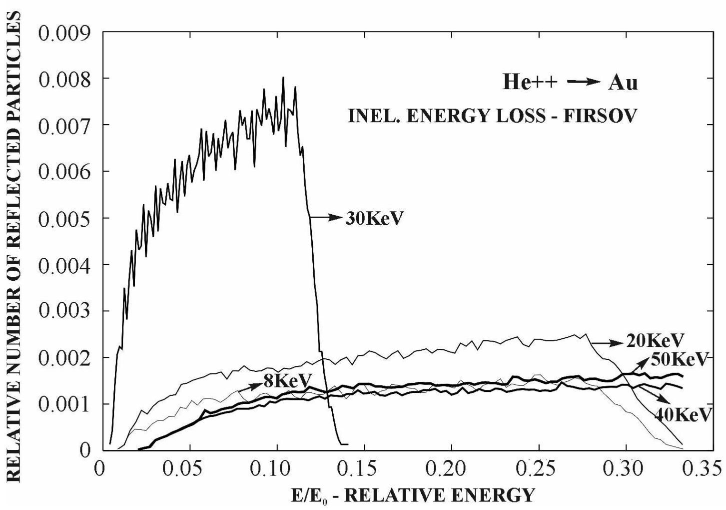


Fig. 3b. Energy distribution of backscattered $He^{2+}$ particles for Firsov.

From Fig. 1a we see that at 8 and 20 keV a great number of particles is backscattered at $\cos\beta \cong 0.52$. Similarly, from Fig. 1b a great number of particles is backscattered a $\cos\beta \cong 0.52$. We expect that BCA is applicable somehow at this exit angles, therefore we drawn Figs. 4a,b, displaying the energy distribution for the LS model for incident energies of 8 and 20 keV (Fig. 4a), and for the F model at 8, 20, and 30 keV (Fig. 4b).

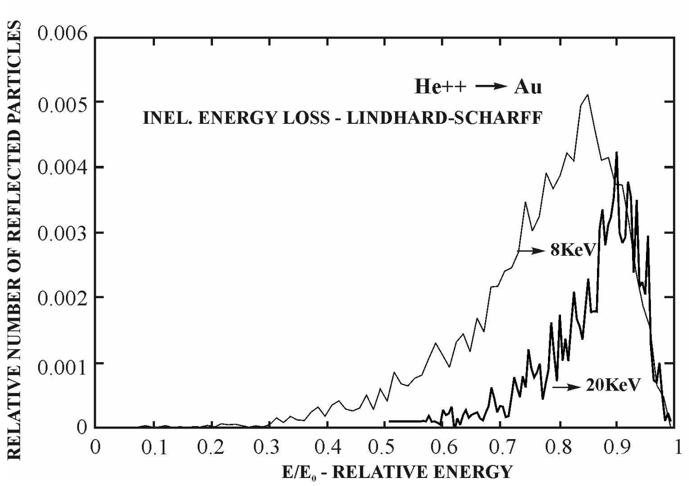


Fig. 4a. Energy distribution of backscattered particles for Lindhard-Scharff parameterization.

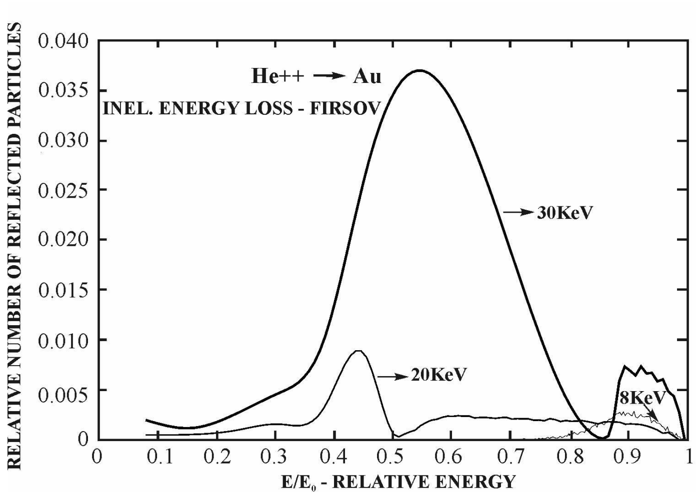


Fig. 4b. Energy distribution of backscattered particles for Firsov parameterization.

The BCA predicts maximums of {0.48; 0.81} for cosβ = 0.52. We see from Figs 3a,b that maximum values occur at $E/E_0 \cong 0.45$, 0.55, 0.83 and 0.93. The discrepancies are due, among others, of course to the fact that we are displaying the integral values of the relative number of backscattered particles.

## 4. Conclusions

We have simulated the backscattering of $He^{++}$ ions from a target consisting in a random assembly of Au atoms for incident energies between 8 and 50 keV and for two models of inelastic energy loss. The results show a sharp distinction in the behavior of 30 keV incident ions, in the sense they 'approach' the BCA. Considering the values predicted by the BCA for the relative number of backscattered particles, we conclude the Firsov model is more accurate to represent the energy loss for this ion - target configuration. Despite the fact that our incident energies are in the range of tens of keV, we suggest the Firsov process is the main responsible mechanism for the energy looses in backscattering events. Further researches will be focused on polycrystalline Au targets as well as on amorphous gold clusters, using adequate interatomic interaction potentials.

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